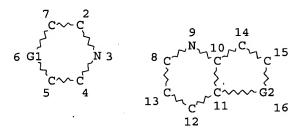
=> d 115 L15 HAS NO ANSWERS L15 STR



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VAR G2=O/S/N
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 8
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

=> s 115 SAMPLE SEARCH INITIATED 14:21:10 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 9691 TO ITERATE

20.6% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 187920 TO 199720 PROJECTED ANSWERS: 2015 TO 3411

L16 28 SEA SSS SAM L15

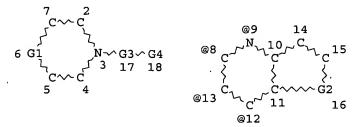
=> s l15 ful FULL SEARCH INITIATED 14:21:15 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 193383 TO ITERATE

100.0% PROCESSED 193383 ITERATIONS 2456 ANSWERS SEARCH TIME: 00.00.01

28 ANSWERS

L17 2456 SEA SSS FUL L15

=> d l18 L18 HAS NO ANSWERS L18 STR



VAR G1=C/N
VAR G2=O/S/N
REP G3=(1-3) A
VAR G4=9/8/13/12
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 8 NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

=> search 118
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:sss
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:subset
ENTER SUBSET L# OR (END):117
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):ful
FULL SUBSET SEARCH INITIATED 14:22:25 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 2456 TO ITERATE

100.0% PROCESSED 2456 ITERATIONS SEARCH TIME: 00.00.01

24 ANSWERS

L19 24 SEA SUB=L17 SSS FUL L18

=> fil caplus TOTAL COST IN U.S. DOLLARS SINCE FILE ENTRY SESSION FULL ESTIMATED COST 214.10 618.18 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -10.14

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FILE COVERS 1907 - 24 Jan 2007 VOL 146 ISS 5 FILE LAST UPDATED: 23 Jan 2007 (20070123/ED)

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http://www.cas.org/infopolicy.html

=> s 119

L20 10 L19

=> d bib abs hitstr 1-10

L20 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:1351110 CAPLUS

DN 144:88316

TI Preparation of azaindoles as inhibitors of p38 kinase

IN Mavunkel, Babu J.; Perumattam, John J.; Lu, Qing; Dugar, Sundeep; Goyal,
Bindu; Wang, Dan X.; Chakravarty, Sarvajit; Luedtke, Gregory R.;
Nashashibi, Imad; Tester, Richland; Tan, Xuefei

PA USA

SO U.S. Pat. Appl. Publ., 83 pp., Cont.-in-part of U.S. Ser. No. 683,656. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	US 2005288299	A1	20051229	US 2005-107027	20050415		
	US 2004176598	A1	20040909	US 2003-683656 ·	20031009		
PRAI	US 2002-417599P	P	20021009				
	US 2003-683656	A2	20031009				
os	MARPAT 144:88316						
GT							

Title compds. [I; dotted line = optional double bond; 1 of Z1, Z2 = CQ, AΒ CR1Q, the other = CRR1, C(R1)2; Q = R1, WiCOXjY; W, X = (substituted)alkylene, alkenylene, alkynylene, heteroalkylene; i, j = 0, 1; Y = COR2, isostere; Z3 = NR7, O, S; Z4, Z5 = N, CH, CR3, or 1 of Z4, Z5 = C to which L1 is linked; \geq 1 of Z4, Z5 = N; Z6 = N, CR5; L1, L2 = (substituted) alkylene, alkenylene, alkynylene, heteroalkylene; Cy = 1-2 (substituted) (fused) 3-7 membered ring(s); R1, R2, R5, R7 = H, R3; R3 = (substituted) alkyl, heteroalkyl, alkenyl, heteroalkenyl, alkynyl, heteroalkynyl, acyl, heteroacyl, aryl, heteroaryl, halo, etc.; R4 = R3, O, NCN, etc.; n = 0-2; m = 0-4; p, q = 0-2; p+k = 0-3], were prepared Thus, title compound (II) inhibited p38 α with IC50 = 0.01 μM . 872355-34-5P 872355-35-6P 872355-36-7P IT 872355-38-9P 872355-39-0P 872355-40-3P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of azaindoles as inhibitors of p38 kinase) RN 872355-34-5 CAPLUS Piperazine, 1-[(4-fluorophenyl)methyl]-2,5-dimethyl-4-(1H-pyrrolo[3,2-CN

Absolute stereochemistry.

RN 872355-35-6 CAPLUS

CN 1H-Pyrrolo[3,2-b]pyridine-3-acetic acid, $5-[[(2R,5S)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-<math>\alpha$ -oxo-, methyl ester (9CI) (CA INDEX NAME)

b]pyridin-5-ylcarbonyl)-, (2S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 872355-36-7 CAPLUS

CN 1H-Pyrrolo[3,2-b]pyridine-3-acetic acid, 5-[[(2R,5S)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-α-οxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 872355-38-9 CAPLUS

CN 1H-Pyrrolo[3,2-b]pyridine-3-acetic acid, 6-chloro-5-[[(2R,5S)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-α-οxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 872355-39-0 CAPLUS

CN Piperazine, 1-[(4-fluorophenyl)methyl]-4-[(6-methoxy-1H-pyrrolo[3,2-b]pyridin-5-yl)carbonyl]-2,5-dimethyl-, (2S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 872355-40-3 CAPLUS

CN Piperazine, 1-[(6-chloro-1H-pyrrolo[3,2-b]pyridin-5-yl)carbonyl]-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-, (2R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 872355-03-8P 872355-04-9P 872355-05-0P 872355-37-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(preparation of azaindoles as inhibitors of p38 kinase)

RN 872355-03-8 CAPLUS

CN 1H-Pyrrolo[3,2-b]pyridine-3-acetamide, 5-[[(2R,5S)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-N-methyl-α-οχο-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 872355-04-9 CAPLUS

CN 1H-Pyrrolo[3,2-b]pyridine-3-acetamide, 6-chloro-5-[[(2R,5S)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-N-methyl- α -oxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 872355-05-0 CAPLUS

CN 1H-Pyrrolo[3,2-b]pyridine-3-acetamide, 5-[[(2R,5S)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-6-methoxy-N-methyl-α-oxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 872355-37-8 CAPLUS

CN 1H-Pyrrolo[3,2-b]pyridine-3-acetic acid, 6-chloro-5-[[(2R,5S)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-α-οχο-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

ethyl ester (9CI) (CA INDEX NAME)

RN 872355-78-7 CAPLUS

CN Piperazine, 1-[(4-fluorophenyl)methyl]-4-[[6-methoxy-1-[[2-(trimethylsilyl)ethoxy]methyl]-1H-pyrrolo[3,2-b]pyridin-5-yl]carbonyl]-2,5-dimethyl-, (2S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 872355-79-8 CAPLUS

CN 1H-Pyrrolo[3,2-b]pyridine-3-acetamide, 5-[[(2R,5S)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-6-methoxy-N-methyl-α-oxo-1-[[2-(trimethylsilyl)ethoxy]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

WO 2004-IB836

os

GI

US 2004-807838

MARPAT 141:314351

Α

A1

20040315

20040323

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L20
    ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
AN
     2004:817865 CAPLUS
DN
     141:314351
     Preparation of 1,2,4-substituted 1,2,3,4-tetrahydro-and 1,2
TI
     dihydro-quinoline and 1,2,3,4-tetrahydro-quinoxaline derivatives as cetp
     inhibitors for the treatment of atherosclerosis and obesity
     Chang, George; Didiuk, Mary Theresa; Finneman, Jari Ilmari; Garigipati,
IN
     Ravi Shanker; Kelley, Ryan Michael; Perry, David Austen; Ruggeri, Roger
     Benjamin; Bechle, Bruce Michael
PΑ
     Pfizer Products Inc., USA
so
     PCT Int. Appl., 335 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
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                         ----
                                _____
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                                                                    _____
ΡI
     WO 2004085401
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                                            WO 2004-IB836
                                                                    20040315
     WO 2004085401
                          A8
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
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             TD, TG
     AU 2004224082
                          A1
                                20041007
                                            AU 2004-224082
                                                                    20040315
    CA 2520405
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                                            CA 2004-2520405
    EP 1622872
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                                20060208
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    BR 2004008897
                          Α
                                20060418
                                            BR 2004-8897
                                                                    20040315
    CN 1795177
                          Α
                                20060628
                                            CN 2004-80014645
                                                                    20040315
                          Т
     JP 2006521344
                                20060921
                                            JP 2006-506369
                                                                    20040315
    US 2004204450
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                                20041014
                                            US 2004-807838
                                                                    20040323
    NL 1025839
                          Α1
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                                                                    20040326
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                          C2
                                20060906
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                          Α
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                                            NO 2005-4989
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    US 2006122224
                          A1
                                20060608
                                            US 2005-305874
                                                                    20051215
                          Ρ
PRAI US 2003-458274P
                                20030328
                          Ρ
    US 2004-536217P
                                20040114
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [X = C; J = N or C, wherein when J = C, then the bond between J and X is a single or double bond, if J = N, then the bond between J and X is a single bond; R1 = Y, W-Z or W-Y; Y = (un)substituted, (un)saturated 3-8 membered ring (or bicyclic ring) optionally having 1-4 heteroatoms, or (un)substituted, (un)saturated 1-10 membered straight or branched carbon chain optionally substituted with 1-2 heteroatoms; W = carbonyl, thiocarbonyl, sulfinyl, or sulfonyl; Z = OY, SY, NHY or NY2; R2 = (un)substituted, (un)saturated 1-6 membered alkyl or heteroalkyl chain; R3 = (un)substituted, (un)saturated alkyl or heteroalkyl chain; R4, R5, R6, and R7 independently = H, bond, nitro, etc.; or adjacent combinations of R4, R5, R6, and R7 may optionally be taken together to form (un)substituted, (un)saturated carbocycle or heterocyclic ring], and pharmaceutical compns. containing such compds. are prepared and disclosed as cholesteryl ester transfer

protein (cetp) inhibitors. Thus, e.g., II was prepared by reaction of 3,5-bistrifluoromethylbenzoyl chloride with 4-diazo-6,7-dimethoxy-2-methyl-3,4-dihydro-2H-quinoline-1-carboxylic acid Et ester (preparation given) in di-Et ether. Methods for bioassaying compds. I are described (no data). The use of I to elevate certain plasma lipid levels, including high d. lipoprotein-cholesterol and to lower certain other plasma lipid levels, such as LDL-cholesterol and triglycerides and accordingly to treat diseases which are exacerbated by low levels of HDL cholesterol and/or high levels of LDL-cholesterol and triglycerides, such as atherosclerosis and cardiovascular diseases in some mammals, including humans is further disclosed.

IT 769128-78-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of quinoline and quinoxaline derivs. as cholesteryl ester transfer protein inhibitors)

RN 769128-78-1 CAPLUS

CN 1(2H)-Quinoxalinecarboxylic acid, 2-ethyl-3,4-dihydro-6,7-dimethyl-4-[[5-(trifluoromethyl)thieno[3,2-b]pyridin-6-yl]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} F_3C & N \\ \hline O & C & S \\ \hline Me & N & Et \\ \hline C - OEt \\ \hline O & C & S \\ \hline \end{array}$$

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:417748 CAPLUS

DN 139:6858

```
Preparation of 1H-pyrrolo[3,2-b]pyridine-3-carboxylic acid amides as GABAA
ΤI
     receptor ligands
IN
     Maynard, George D.; Ghosh, Manuka; O'Donnell, Christopher J.
PA
     Neurogen Corporation, USA
SO
     PCT Int. Appl., 134 pp.
     CODEN: PIXXD2
DT
     Patent
     English
T.A
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                             APPLICATION NO.
                                                                    DATE
PΙ
     WO 2003044018
                          A1
                                 20030530
                                             WO 2002-US37157
                                                                     20021119
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                20030530
                                            CA 2002-2467542
     CA 2467542
                          Α1
                                                                     20021119
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                                             AU 2002-366092
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     EP 1453831
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                                                                     20021119
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     BR 2002014301
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                          Α
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     JP 2005516901
                          Т
                                             JP 2003-545655
                                20050609
                                                                     20021119
PRAI US 2001-333027P
                          Р
                                20011119
     WO 2002-US37157
                          W
                                20021119
     MARPAT 139:6858
os
GI
```

AB Disclosed are 1H-pyrrolo[3,2-b]pyridine-3-carboxylic acid amides (shown as I; variables defined below; e.g. 5-(1-Methylpiperidin-4-yloxy)-1Hpyrrolo[3,2-b]pyridine-3-carboxylic acid pyridin-2-ylamide) that bind to the benzodiazepine site of GABAA receptors. Such compds. can be used to modulate ligand binding to GABAA receptors in vivo and in vitro, and are particularly useful in the treatment of a variety of central nervous system (CNS) disorders in humans, domesticated companion animals, and livestock animals. Each of 120 examples of I was tested for binding to the benzodiazepine site of GABAA receptors and each has a Ki of <4 µM; preferred compds. exhibit Ki values of <100 nM and more preferred compds. exhibit Ki values of <10 nM; individual values are not given. Although the methods of preparation are not claimed, 2 example prepns. and characterization data for .apprx.120 examples of I are included. For I: R1, R2, and R3 = H, halogen, halo(C1-C6)alkyl, hydroxy, cyano, amino, alkyl, alkoxy, mono- or di-(C1-C6)alkylamino, mono- or

di-(C1-C6)alkylamino(C1-C6)alkyl, -C(0)NR10R11, -C(0)OR10, and -OC(0)R10,
-C(0)R10 (R10 and R11 = H, C1-C6 alkyl, Ph, phenyl(C1-C6)alkyl, pyridyl,
or pyridyl(C1-C6)alkyl), haloalkoxy, alkenyl, alkynyl, hydroxyalkyl,
-D-R20, -E-R35, -C1-C4alkyl-D-R20, -C1-C4alkyl-O-R20, -E-R20-G-R30, -E-L,
-E-R20-L, J, -C(0)-L, or -C1-C4alkyl-J. D is -S(0)n-, -S(0)nNH-,
-S(0)nNH2, -S(0)nNR30-, -NHC(0)-, -NHC(0)H, -NR30C(:0)-, -NR30C(:0)H,
-NHS(0)n-, and -NR30S(0)n-; E and G = -NH-, -N(C1-C6alkyl)-, S, and O;
each R20 and R30 = (C1-C8)alkyl, (C3-C8) cycloalkyl or
(C3-C8)cycloalkyl(C1-C6)alkyl; each R35 = (C1-C8)straight, (C1-C8)
branched, (C3-C8)cyclic alkyl or (C3-C8) cycloalkyl(C1-C6)alkyl; J and L =
saturated, partially unsatd., and aromatic rings having 4-7 ring atoms, where

1, or 2 of the ring atoms are 0 or N and the remaining ring atoms are C,
where the rings are (un)substituted with ≥1 substituents. R4 is H,
halogen, or hydroxy; Ar = aryl, arylalkyl, heteroarylalkyl or heteroaryl
group; each n = 0, 1, or 2; addnl. details including provisos are given in
the claims. A method using compds. I and autoradiog. is claimed for
determining

the presence or absence of GABAA receptor in a sample. IT 533912-89-9P, 5-[2-(4-Methylpiperazin-1-yl)ethoxy]-1H-pyrrolo[3,2b]pyridine-3-carboxylic acid pyridin-2-ylamide 533912-91-3P, 5-[2-(4-Methylpiperazin-1-yl)ethoxy]-1H-pyrrolo[3,2-b]pyridine-3carboxylic acid (1-methyl-1H-pyrazol-3-yl)amide RL: ARG (Analytical reagent use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate and anal. reagent; preparation of pyrrolopyridinecarboxamides as GABAA receptor ligands) 533912-89-9 CAPLUS RN CN 1H-Pyrrolo[3,2-b]pyridine-3-carboxamide, 5-[2-(4-methyl-1piperazinyl)ethoxy]-N-2-pyridinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & H \\
 & N \\
 & C \\
 & N \\$$

RN 533912-91-3 CAPLUS
CN 1H-Pyrrolo[3,2-b]pyridine-3-carboxamide, 5-[2-(4-methyl-1-piperazinyl)ethoxy]-N-(1-methyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & H & O \\
 & N & CH_2 - CH_2 - O \\
 & N & C - NH \\
\end{array}$$
Me

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:324914 CAPLUS

DN 137:379663

0,

TI Identification of potent and selective oxytocin antagonists. Part 1: indole and benzofuran derivatives

- AU Wyatt, Paul G.; Allen, Michael J.; Chilcott, Josie; Foster, Alison; Livermore, David G.; Mordaunt, Jackie E.; Scicinski, Jan; Woollard, Patrick M.
- CS Department of Medicinal Chemistry, Medicines Research Centre, GlaxoSmithKline, Herts, Stevenage, SG1 2NY, UK
- SO Bioorganic & Medicinal Chemistry Letters (2002), 12(10), 1399-1404 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- OS CASREACT 137:379663
- AB Studies to discover novel, potent and selective oxytocin antagonists are reported. Combinatorial libraries designed to find novel replacements of fragments of oxytocin antagonist L-371,257, identified pyrimidine, thiazole, indole and benzofuran as potential alternatives to the benzoic acid moiety of L-371,257. Addnl. investigations identified indole and benzofuran derivs. with potent oxytocin antagonist activity.
- IT 475649-73-1
 - RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 - (preparation and structure activity relationship of benzofuran derivs. as oxytocin antagonists)
- RN 475649-73-1 CAPLUS
- CN Piperidine, 4-(2-oxo-2H-3,1-benzoxazin-1(4H)-yl)-1-(1H-pyrrolo[3,2-b]pyridin-5-ylcarbonyl)- (9CI) (CA INDEX NAME)

- RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L20 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2002:157780 CAPLUS
- DN 136:216748
- TI Preparation of 1H-imidazopyridine derivatives as TNF and interleukin-1 production inhibitors
- IN Kato, Hideo; Sakaguchi, Jun; Izumi, Tomoyuki; Kato, Kenichi
- PA Hokuriku Seiyaku Co., Ltd., Japan
- SO PCT Int. Appl., 76 pp. CODEN: PIXXD2
- DT Patent
- LA Japanese
- FAN.CNT 1

	PATEN	T NO.	NO.			KIND DATE				APPLICATION NO.						DATE 20010821		
ΡI	WO 20	70		<i></i> - A1 2			20020228			WO 2001-JP7150								
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		GM,	HR,	HU,	ID,	IL,	IN,	IS,	KE,	KG,	KR,	KZ,	LC,	LK,	LR,	LS,	LT.	

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             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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                          A5
                                20020304
PRAI JP 2000-250874
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                                20000822
     JP 2001-116240
                          Α
                                20010416
     WO 2001-JP7150
                          W
                                20010821
os
     MARPAT 136:216748
GI
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AB The title compds. I [R1 is hydrogen, alkyl, cycloalkyl, or aryl; R2 is hydrogen or lower alkyl; R3 is a saturated nitrogenous heterocyclic group; m is an integer of 0 to 3; and ring A is, e.g., an (un)substituted thiophene ring, etc., (said thiophene ring is fused to the pyridine ring)] are prepared In an in vitro test using cells, 4-methyl-1-[2-(4-piperidyl)ethyl]-2-(2-pyrrolyl)-1H-imidazo[5,4-d]thieno[3,2-b]pyridine at 0.001 μmol/L gave 73% inhibition of TNF-α production

IT 402566-81-8P 402566-91-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 1H-imidazopyridine derivs. as TNF and interleukin-1 production

inhibitors)

RN 402566-81-8 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-[(5-methyl-6-nitrothieno[3,2-b]pyridin-7-yl)amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 402566-91-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-[(6-amino-5-methylthieno[3,2-b]pyridin-7-yl)amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2001:762989 CAPLUS

DN 135:318419

TI Synthesis of substituted bipiperidines and their use as H1 antagonists

IN Lawrence, Louise; Rigby, Aaron; Sanganee, Hitesh; Springthorpe, Brian

PA Astrazeneca AB, Swed.

SO PCT Int. Appl., 160 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.

KIND DATE

APPLICATION NO.

DATE

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WO 2001077101
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             HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
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     EP 2001-920053
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                                 20010405
     WO 2001-SE751
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     US 2001-827488
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     US 2003-341027
                          A1
                                 20030113
     US 2003-436582
                          Α3
                                 20030513
os
     MARPAT 135:318419
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GI

AB Title compds. I [q, s, t = 0 - 1; n, r = 0 - 5; m, p = 0 - 2; X = CH, C(0), O, S, S(0), S(0), N-; provided that when m and p are both 1 then X is not CH; Y = NHR2, OH; T = C(0), C(S), S(0), CH2; R1 = H, alkyl, aryl, heterocyclyl; R2, R47 = H, alkyl, aryl-alkyl, CO-alkyl; R3 = alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, heterocyclyl, thioaryl, thioheterocyclyl] were prepared Examples include: data for over 600 compds., 4 solid oral dosage and 1 parenteral (general) formulations, a bioassay for Ca2+ flux, human eosinophil chemotaxis and H1 antagonism. E.g., 4-(3,4-dichlorophenoxy)piperidine was alkylated with 1-(tert-butoxycarbonyl)-4-piperidone (1,2-dichloroethane, NaBH(OAc)3, HOAc, 18 h, room temperature) to give an intermediate [1,4']bipiperidine. This intermediate was deprotected (DCM, TFA, 4 h, room temperature) and the resulting

ΙI

bipiperidine condensed with 3-methanesulfonylbenzoic acid (THF, PYBROP, (i-Pr)2NEt, 18 h, room temperature) to give example compound II isolated as the acetate salt. I are used in the treatment of a chemokine (such as CCR3) or H1 mediated disease state.

IT 367498-32-6P 367499-96-5P 367499-97-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug; synthesis of substituted bipiperidines and use as H1
 antagonists)

RN 367498-32-6 CAPLUS

$$\begin{array}{c|c} & & & & \\ & &$$

RN 367499-96-5 CAPLUS

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 367499-97-6 CAPLUS

CN 1,4'-Bipiperidine, 4-(4-chloro-3-methylphenoxy)-1'-[[5-(trifluoromethyl)thieno[3,2-b]pyridin-6-yl]carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2001:78383 CAPLUS

DN 134:163059

TI Substituted piperazinone derivatives and other oxoazaheterocyclyl compounds useful as factor Xa/IIa inhibitors

IN Ewing, William R.; Becker, Michael R.; Choi-Sledeski, Yong Mi; Pauls,
Heinz W.; He, Wei; Condon, Stephen M.; Davis, Roderick S.; Hanney, Barbara
A.; Spada, Alfred P.; Burns, Christopher J.; Jiang, John Z.; Li, Aiwen;
Myers, Michael R.; Lau, Wan F.; Poli, Gregory B.

PA Aventis Pharmaceuticals Products Inc., USA

SO PCT Int. Appl., 460 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 3

PATENT NO. KIND DATE APPLICATION NO. DATE _____ PΙ WO 2001007436 A2 20010201 WO 2000-IB1156 20000726 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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	BR	2000	0131	79		Α	200	20402	BR	2000-	1317	9	20000			726		
	EP	P 1208097				A2	200	20529	EP 2000-951781					20000726				
		R:	ΑT,	BE,	CH,	DE,	DK, ES	, FR,	GB, GF	R, IT,	LI,	LU,	NL,	SE,	MC,	PT,		
			IE,	SI,	ĻΤ,	LV,	FI, RO	, MK,	CY, AI									
	TR	2002	0022	5		T2	200	20621	TR	2002-	225			2	0000	726		
	HU	2002	0337	5		A2	200	21228	HU	2002-	3375			2	0000	726		
	JP	2003	5083	53		T	200	30304	JP	2001-	5125	20		2	0000	726		
	$\mathbf{E}\mathbf{E}$	2002	0004	5		Α	200	30616	EE	2002-	45			2	0000	726		
	ΑU	7732	27			B2	200	40520	AU	2000-	6462	8		2	0000	726		
	ИО	2002	0002	14		Α	200	20402	ИО	2002-	214			2	0020	115		
	BG	1063	40			Α	200	21031	BG	2002-	1063	40		2	0020	122		
	ZA	2002	0005	43		Α	200	30623	ZA	2002-	543			2	0020	122		
PRAI	US	1999	-363	196		Α	199	90728										
	WO	2000	-IB1	156		W	200	00726										
os	MAF	RPAT	134:	1630	59													
GT																		

Ι

AΒ The invention is directed to piperazinones I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates [wherein A = CH or N; G1 and G2 = L1Cy1 or L2Cy2; Cy1 and Cy2 = (un)substituted aryl, heteroaryl, cycloalkyl, cycloalkenyl, heterocyclyl, etc.; L1 = null, O, S, SO, SO2, or (un) substituted sulfamoyl, methylene, (alkyl) keto(alkyl), carbamoyl, etc.; L2 = null or linking group; R1, R1a, R2, R2a, R3, R3a, R4, R4a = independently H, carboxy, alkoxycarbonyl, alkyl, (hetero)aryl, aralkyl, heteroarylalkyl, etc.; m and n = independently 0-2]. The compds. inhibit factor Xa (no data) and factor IIa, and thereby the production of thrombin, and are thus useful as anticoagulants in the treatment of a wide variety of conditions. The invention is also directed to pharmaceutical compns., synthetic intermediates, and a method of inhibiting factor Xa. Examples include the synthesis of approx. 1600 invention compds. and several hundred intermediates. For instance, condensation of 5-chloro-2-thienyloxyacetic acid with the corresponding N-benzyloxycarbonyl-protected piperazinone derivative (prepns. given), using DIPEA and TBTU in DMF, gave II.

II

IT 234102-19-3P

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of piperazinone derivs. and other substituted oxoazaheterocyclyl compds. as factor Xa/IIa inhibitors)

RN 234102-19-3 CAPLUS

Piperazinone, 1-[(4-amino-7-quinazoliny1)methy1]-4-[(5-chlorothieno[3,2-

$$\begin{array}{c|c} & & & \\ & & & \\$$

L20 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2000:576158 CAPLUS

DN 133:275852

TI Identification of MK-944a: A Second Clinical Candidate from the Hydroxylaminepentanamide Isostere Series of HIV Protease Inhibitors

AU Dorsey, Bruce D.; McDonough, Colleen; McDaniel, Stacey L.; Levin, Rhonda B.; Newton, Christina L.; Hoffman, Jacob M.; Darke, Paul L.; Zugay-Murphy, Joan A.; Emini, Emilio A.; Schleif, William A.; Olsen, David B.; Stahlhut, Mark W.; Rutkowski, Carrie A.; Kuo, Lawrence C.; Lin, Jiunn H.; Chen, I-W.; Michelson, Stuart R.; Holloway, M. Katharine; Huff, Joel R.; Vacca, Joseph P.

CS Departments of Medicinal Chemistry Antiviral Research Drug Metabolism and Molecular Systems, Merck Research Laboratories, West Point, PA, 19486, USA

SO Journal of Medicinal Chemistry (2000), 43(18), 3386-3399 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

OS CASREACT 133:275852

Recent results from human clin. trials have established the critical role of AB HIV protease inhibitors in the treatment of acquired immune-deficiency syndrome (AIDS). However, the emergence of viral resistance, demanding treatment protocols, and adverse side effects have exposed the urgent need for a second generation of HIV protease inhibitors. The continued exploration of the authors hydroxylaminepentanamide (HAPA) transition-state isostere series of HIV protease inhibitors, which initially resulted in the identification of Crixivan (indinavir sulfate, MK-639, L-735,524), has now yielded MK-944a (L-756,423). This compound is potent, is selective, and competitively inhibits HIV-1 PR with a Ki value of 0.049 nM. It stops the spread of the HIVIIIb-infected MT4 lymphoid cells at 25.0-50.0 nM, even in the presence of $\alpha 1$ acid glycoprotein, human serum albumin, normal human serum, or fetal bovine serum. MK-944a has a longer half-life in several animal models (rats, dogs, and monkeys) than indinavir sulfate and is currently in advanced human clin. trials. 298702-87-1P

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(identification of MK-944a as second clin. candidate from hydroxylaminepentanamide isostere series of HIV protease inhibitors with good bioavailability and pharmacokinetics and low toxicity in relation to antiviral resistance)

RN 298702-87-1 CAPLUS

CN D-erythro-Pentonamide, 2,3,5-trideoxy-N-[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]-5-[(2S)-2-[[(1,1-dimethylethyl)amino]carbonyl]-4-(furo[3,2-b]pyridin-6-ylmethyl)-1-piperazinyl]-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

WO 1999-US1682

US 1999-313611

US 1999-363196

US 1998-72707P

os

GΙ

WO 1999-US28074

MARPAT 133:30741

A2

A2

A2

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W

19990127

19990518

19990728

19980127

19991124

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN L20 AN2000:384179 CAPLUS DN 133:30741 Substituted piperazinone derivatives and other oxoazaheterocyclyl TI compounds useful as factor Xa inhibitors IN Ewing, William R.; Becker, Michael R.; Myers, Michael R.; Spada, Alfred P. PA Aventis Pharmaceuticals Products Inc., USA SO PCT Int. Appl., 219 pp. CODEN: PIXXD2 DT Patent LA English FAN.CNT 3 PATENT NO. KIND DATE APPLICATION NO. DATE · - - - - - - - - - - - - - - ------WO 2000032590 20000608 WO 1999-US28074 PΙ A1 19991124 AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP; KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG WO 9937304 19990729 WO 1999-US1682 **A1** 19990127 AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, GW, ML, MR, NE, SN, TD, TG CM, GA, GN, JP 2003529531 20031007 JP 2000-585232 \mathbf{T} 19991124 PRAI US 1998-110012P Α2 19981125

AB The invention is directed to piperazinones I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates [wherein R1 = H, alkyl, aryl, aralkyl, heteroaryl, heteroarylalkyl, alkoxy, aminoalkyl, CH2OZ, CH(CH3)OZ; R2 = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl, or heteroarylalkyl; R3 = H or Me; X = N or O; Z = lower alkyl or alkoxycarbonylalkyl; Cy1 = (un)substituted aryl, (un)substituted heteroaryl; Cy2 = (un) substituted aryl, heteroaryl, cycloalkyl, cycloalkenyl, heterocyclyl, etc.]. The compds. inhibit factor Xa (no data), and thereby the production of thrombin, and are thus useful as anticoagulants in the treatment of a wide variety of conditions. invention is also directed to pharmaceutical compns., synthetic intermediates, and a method of inhibiting factor Xa. Examples include the synthesis of approx. 780 invention compds., approx. 50 of which are also claimed, and several hundred intermediates. For instance, condensation of 5-chloro-2-thienyloxyacetic acid with the corresponding N-benzyloxycarbonyl-protected piperazinone derivative (prepns. given), using DIPEA and TBTU in DMF, gave the preferred title compound II. TΤ 234102-19-3P

II

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of piperazinone derivs. and other substituted oxoazaheterocyclyl compds. as factor Xa inhibitors)

RN 234102-19-3 CAPLUS

CN

Piperazinone, 1-[(4-amino-7-quinazolinyl)methyl]-4-[(5-chlorothieno[3,2-b]pyridin-6-yl)methyl]- (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN AN 1999:487215 CAPLUS

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Substituted piperazinone derivatives and other oxoazaheterocyclyl
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     compounds useful as factor Xa inhibitors
     Ewing, William R.; Becker, Michael R.; Choi-Sledeski, Yong Mi; Pauls,
IN
     Heinz W.; He, Wei; Condon, Stephen M.; Davis, Roderick S.; Hanney, Barbara
     A.; Spada, Alfred P.; Burns, Christopher J.; Jiang, John Z.; Li, Aiwen;
     Myers, Michael R.; Lau, Wan F.; Poli, Gregory B.
     Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
PΑ
SO
     PCT Int. Appl., 300 pp.
     CODEN: PIXXD2
DT
     Patent
     English
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     PATENT NO.
                         KIND
                                DATE
                                           APPLICATION NO.
                                                                    DATE
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                                19990729
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             LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT,
             RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ,
             VN, YU, ZW
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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     EP 1051176
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             IE, SI, LT, LV, FI, RO
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                                                                    19990127
     JP 2002501024
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                          A1
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             UG, US, UZ, VN, YU, ZW
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
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     JP 2003529531
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    BG 104633
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                          Α1
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PRAI US 1998-72707P
                          A2
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                                19981125
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                          W
                                19990127
    US 1999-313611
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                                19990518
    US 1999-363196
                          A2
                                19990728
    WO 1999-US28074
                          W
                                19991124
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    MARPAT 131:130007
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131:130007

AB The invention is directed to oxoazaheterocyclyl compds. I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates [wherein A = CH, N; G1, G2 = (independently) -L-Cy; L = various atomic and mol. linkers, including O, (un) substituted NH or S, alk(en/yn)ylene, etc., or their combinations; Cy = (un)substituted (hetero)aryl, cycloalk(en)yl, heterocyclyl, etc.; R = (independently) H, CO2H, alkoxycarbonyl, (un)substituted carbamoyl, alkyl, (hetero)aryl, (hetero)aralkyl; or two geminal R groups = 0 or S; m, n = 0-2; with provisos]. The compds. inhibit factor Xa (no data), and thereby the production of thrombin, and are thus useful as anticoagulants in the treatment of a wide variety of conditions. The invention is also directed to pharmaceutical compns., synthetic intermediates, and a method of inhibiting factor Xa. Examples include the synthesis of approx. 780 compds. I, which are also claimed, and several hundred intermediates. instance, sulfonamidation of 6-chlorobenzo[b]thiophene-2-sulfonyl chloride with 4-(2-oxopiperazin-1-ylmethyl) benzamidine bistrifluoroacetate (prepns. given) in CH2Cl2 in the presence of Et3N gave title compound II. 234102-19-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of piperazinone derivs. and other substituted oxoazaheterocyclyl compds. as factor Xa inhibitors)

RN 234102-19-3 CAPLUS

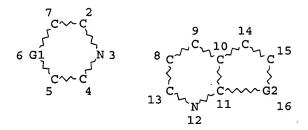
CN

Piperazinone, 1-[(4-amino-7-quinazolinyl)methyl]-4-[(5-chlorothieno[3,2-b]pyridin-6-yl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\$$

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 16 L6 HAS NO ANSWERS



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GRAPH ATTRIBUTES:
RSPEC 8
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

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24.2% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

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L7 50 SEA SSS SAM L6

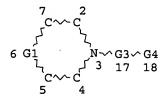
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100.0% PROCESSED 165556 ITERATIONS , 6958 ANSWERS SEARCH TIME: 00.00.01

50 ANSWERS

L8 6958 SEA SSS FUL L6

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100.0% PROCESSED 6958 ITERATIONS SEARCH TIME: 00.00.01

293 ANSWERS

L12. 293 SEA SUB=L8 SSS FUL L11

=> d scan

Absolute stereochemistry.

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L3			STR						
L4	(39)	SEA	FILE=	REGIS	TRY	SSS	FUL	L3
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L7 50 S L6 L8 6958 S L6 FUL

FILE 'CAPLUS' ENTERED AT 14:01:18 ON 24 JAN 2007 861 S L8

L9 861 S L8 L10 172 S L9 AND INFLAMMA?

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L11 STRUC

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FILE 'CAPLUS' ENTERED AT 14:03:37 ON 24 JAN 2007

L13 59 S L12

L14 43 S L13 AND PY<2002

=> d bib abs hitstr 1

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ANSWER 1 OF 43 CAPLUS COPYRIGHT 2007 ACS on STN
     2001:935602 CAPLUS
AN
DN
     136:69741
ΤI
     Preparation of azaindoles as antitumor agents
     Longo, Antonio; Brasca, Maria Gabriella; Orsini, Paolo; Traquandi,
ΤN
     Gabriella; Pittala, Valeria; Vulpetti, Anna; Varasi, Mario; Pevarello,
     Paolo
     Pharmacia & Upjohn S.p.A., Italy
PA
     PCT Int. Appl., 150 pp.
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     CODEN: PIXXD2
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     Patent
    English
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                                            APPLICATION NO.
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    WO 2001098299
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                         A1
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    US 2003004350
                          A1
                                20030102
PRAI US 2000-597274
                          Α
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     WO 2001-EP6890
                          W
                                20010613
     MARPAT 136:69741
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$$R^2$$
 R^3
 R^1
 R^1

Ι

AB The title 1H-pyrrolo[2,3-b]pyridines [I; R = H, halo, CN, etc.; R1 = H, alkyl; R2 = alkyl, aryl; R3 = H, CONR4R5, CO2R4, CONHOR4, SO2NHR4, alkylsulfonylaminocarbonyl, perfluorinated alkylsulfonylaminocarbonyl; R4, R5 = H, alkyl, aryl, etc.] or their pharmaceutically acceptable salts, useful for treating cell proliferative disorders associated with an altered cell cycle dependent kinase activity (no data given), were prepared Thus,

reacting phenylacetic acid with 1H-pyrrolo[2,3-b]pyridine-3-carbaldehyde in the presence of Ac2O and Et3N afforded 44% I [R, R1 = H; R2 = Ph; R3 = CO2H].

IT 383869-91-8P 383869-93-0P 383870-60-8P
383870-64-2P 383871-25-8P 383871-27-0P
383872-04-6P 383872-06-8P 383872-52-4P
383872-55-7P 383872-92-2P 383872-94-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azaindoles as antitumor agents)

RN 383869-91-8 CAPLUS CN 1-Piperidinecarboxar

1-Piperidinecarboxamide, N-[3-(3-amino-3-oxo-2-phenyl-1-propenyl)-1H-pyrrolo[2,3-b]pyridin-6-yl]- (9CI) (CA INDEX NAME)

=> d bib abs hit hitstr 38

CASREACT 113:115227

OS

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The treatment of 2-thioxo-1,2-dihydropyridine-3-carbonitriles with ClCH2CO2NR1R3 (R1, R2 = H, Me, Et) gave 3-aminothieno[2,3-b]pyridinecarboxylic acid amides I [R1 = H, Et, Me, R2 = H, Et, Bu, cyclohexyl, CH2CH2OH, CH2CO2H; R1R2 = (CH2)5; R3 = Me, Ph, 4-BrC6H4, 3-pyridyl, CONH2, etc; R4 = H, Me, CH2C6H4(CN)-4; R5 = Me, C6H4Cl-4, Ph, C6H4Br-4, furyl, naphthyl, OH). Some of the compds. thus prepared, e.g. I (R1 = R2 = R4 = H, R3 = Me, R5 = Ph) and I (R1 = R4 = H, R2 = CH2CH2OH, R3 = R5 = Me) showed activity as antiallergics in the passive cutaneous anaphylaxis test in rats.

SO Pharmazie (1990), 45(2), 102-9 CODEN: PHARAT; ISSN: 0031-7144

I

67795-42-0P IT 56891-69-1P 72701-64-5P 94638-98-9P 115919-79-4P 119003-35-9P 119003-36-0P 115919-80-7P 115919-86-3P 119003-37-1P 119003-38-2P 119003-39-3P 128917-96-4P 128917-97-5P 128917-98-6P 128917-99-7P 128918-00-3P 128918-01-4P 128918-02-5P 128918-03-6P 128918-06-9P 128918-04-7P 128918-05-8P 128918-07-0P 128918-08-1P 128918-09-2P 128918-10-5P 128918-11-6P 128918-13-8P 128918-15-0P 128918-16-1P 128918-17-2P 128918-18-3P 128918-19-4P 128918-20-7P 128918-21-8P 128918-22-9P 128918-23-0P 128918-24-1P 128918-25-2P 128918-26-3P 128918-27-4P 128918-28-5P 128918-29-6P 128918-30-9P 128918-31-0P 128918-33-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

IT 128918-08-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

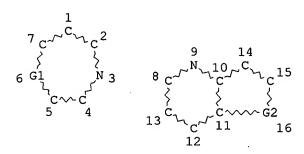
RN 128918-08-1 CAPLUS

CN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-methyl-4-(1piperidinylcarbonyl)- (9CI) (CA INDEX NAME)

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$$Me \qquad N$$

=> d 14 L4 HAS NO ANSWERS L4 STR



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VAR G2=O/S/N
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 1 8

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

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BATCH **COMPLETE**

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100.0% PROCESSED 199413 ITERATIONS

SEARCH TIME: 00.00.02

L6 39 SEA SSS FUL L4

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L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(4S)-hexahydro-1-(4-morpholinylsulfonyl)-3-oxo-1H-azepin-4-yl]amino]carbonyl]-3-methylbutyl]-3-methyl- (9CI)

MF C25 H35 N5 O7 S

Absolute stereochemistry.

0 ANSWERS

39 ANSWERS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):38

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(4S,7R)-hexahydro-2,4-d2-7-methyl-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl-2-d]amino]carbonyl]-3-methylbutyl]-3-methyl- (9CI)

MF C27 H30 D3 N5 O6 S

Absolute stereochemistry.

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[(4S,7R)-hexahydro-7-methyl-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]amino]-2-oxoethyl]-3-methyl- (9CI)

MF C30 H37 N5 O6 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C14 H19 N3 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[3,2-b]pyridine, 7-(hexahydro-1H-1,4-diazepin-1-yl)-5-phenyl- (9CI)

MF C18 H19 N3 S

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C29 H27 F N4 O3 S2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C14 H16 N4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2[[(3S,4S,7R)-hexahydro-3-hydroxy-7-methyl-1-(2-pyridinylsulfonyl)-1Hazepin-4-yl]amino]-2-oxoethyl]-3-methyl- (9CI)

MF C30 H39 N5 O6 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(4S,7R)-hexahydro-2,4-d2-7-methyl-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl-2-d]amino]carbonyl]-3-methylbutyl]- (9CI)

MF C26 H28 D3 N5 O6 S

Absolute stereochemistry.

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Azepin-3-amine, 1-furo[3,2-b]pyridin-6-ylhexahydro-, (3R)- (9CI)

MF C13 H17 N3 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxamide, hexahydro-N-methyl-4-(5-phenylthieno[3,2-b]pyridin-7-yl)- (9CI)

MF C20 H22 N4 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C28 H34 F3 N3 O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[hexahydro-1-[(1-oxido-2pyridinyl)sulfonyl]-3-oxo-1H-azepin-4-yl]amino]carbonyl]-3-methylbutyl]-3methyl- (9CI)

MF C26 H31 N5 O7 S

Absolute stereochemistry.

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[1-[[((4S,7R)-hexahydro-7-methyl-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]amino]carbonyl]cyclohexyl]-3-methyl- (9CI)

MF C28 H33 N5 O6 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Azepin-4-amine, 1-furo[3,2-b]pyridin-6-ylhexahydro-, (4R)- (9CI)

MF C13 H17 N3 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxamide, N-ethylhexahydro-4-(5-phenylthieno[3,2-b]pyridin-7-yl)- (9CI)

MF C21 H24 N4 O S

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[3,2-b]pyridine-3-carbonitrile, 2-[[2-(hexahydro-1H-azepin-1-yl)ethyl]thio]-4,5-dihydro-7-hydroxy-5-oxo- (9CI)

MF C16 H19 N3 O2 S2

$$S$$
 S CH_2 CH_2 N CN

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[3,2-b]pyridine-3-carbonitrile, 2-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)- (9CI)

MF C14 H17 N5

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[1-[[[(45,7R)-hexahydro-3-hydroxy-7-methyl-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]amino]carbonyl]cyclohexyl]-3-methyl- (9CI)

MF C28 H35 N5 O6 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1 \S)-1-[[[(4 \S ,7R)-hexahydro-7-methyl-3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]amino]carbonyl]-3-methylbutyl]-3-methyl- (9CI)

MF C27 H33 N5 O6 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

1H-Azepin-3-amine, 1-furo[3,2-b]pyridin-6-ylhexahydro-N-methyl-, (3R)-IN (9CI)

C14 H19 N3 O MF

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN L6

Thieno[3,2-b]pyridine, 7-(hexahydro-1H-1,4-diazepin-1-yl)-5-phenyl-, IN

dihydrochloride (9CI) C18 H19 N3 S . 2 Cl H MF

●2 HCl

L639 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[3,2-b]pyridine, 1-[(1S)-1-[(hexahydro-1H-azepin-1yl)methyl]propyl]-5-[2-methoxy-4-(trifluoromethoxy)phenyl]-3,6-dimethyl-(9CI)

C27 H34 F3 N3 O2 MF

Absolute stereochemistry.

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[(4R)-hexahydro-1-[(1-oxido-2-pyridinyl)sulfonyl]-3-oxo-1H-azepin-4-yl]amino]carbonyl]-3-methylbutyl]-(9CI)

MF C25 H29 N5 O7 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(3S,4S,7R)-hexahydro-3-hydroxy-7-methyl-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]amino]carbonyl]-3-methylbutyl]-3-methyl- (9CI)

MF C27 H35 N5 O6 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C14 H19 N3 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Azepin-3-amine, 1-furo[3,2-b]pyridin-6-ylhexahydro-, (3S)- (9CI)
MF C13 H17 N3 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[3,2-b]pyridine, 3-(4-fluorophenyl)-1-[3-(hexahydro-1H-1,4-diazepin-1-yl)propyl]-2-(4-pyridinyl)- (9CI)

MF C26 H28 F N5

CI COM

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(4S,7R)-hexahydro-7-methyl1-(4-morpholinylsulfonyl)-3-oxo-1H-azepin-4-yl]amino]carbonyl]-3methylbutyl]-3-methyl- (9CI)

MF C26 H37 N5 O7 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(3S,4S,7R)-hexahydro-3-hydroxy-7-methyl-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]amino]carbonyl]-3-methylbutyl]- (9CI)

MF C26 H33 N5 O6 S

Absolute stereochemistry.

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(4S,7R)-hexahydro-7-methyl1-[(1-oxido-2-pyridinyl)sulfonyl]-3-oxo-1H-azepin-4-yl]amino]carbonyl]-3methylbutyl]-3-methyl- (9CI)

MF C27 H33 N5 O7 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Azepin-4-amine, 1-furo[3,2-b]pyridin-6-ylhexahydro-, (4S)- (9CI)

MF C13 H17 N3 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxamide, N-ethylhexahydro-4-(5-phenylthieno[3,2-b]pyridin-7-yl)-, dihydrochloride (9CI)

MF C21 H24 N4 O S . 2 Cl H

●2 HCl

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzeneacetamide, N-[[[3-fluoro-4-[[2-[(hexahydro-1H-azepin-1-yl)carbonyl]thieno[3,2-b]pyridin-7-yl]oxy]phenyl]amino]thioxomethyl]-,
 monohydrochloride (9CI)

MF C29 H27 F N4 O3 S2 . C1 H

● HCl

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(4S)-hexahydro-1-[(1-oxido-2-pyridinyl)sulfonyl]-3-oxo-1H-azepin-4-yl]amino]carbonyl]-3-methylbutyl]-(9CI)

MF C25 H29 N5 O7 S

Absolute stereochemistry.

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(3S,4S,7R)-hexahydro-3-hydroxy-7-methyl-1-[(1-oxido-2-pyridinyl)sulfonyl]-1H-azepin-4yl]amino]carbonyl]-3-methylbutyl]-3-methyl- (9CI)

MF C27 H35 N5 O7 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[3,2-b]pyridine-2-carboxamide, N-[(1S)-1-[[[(4S,7R)-hexahydro-7-methyl3-oxo-1-(2-pyridinylsulfonyl)-1H-azepin-4-yl]amino]carbonyl]-3methylbutyl]- (9CI)

MF C26 H31 N5 O6 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Azepin-3-amine, 1-furo[3,2-b]pyridin-6-ylhexahydro-N-methyl-, (3S)(9CI)

MF C14 H19 N3 O

Absolute stereochemistry.

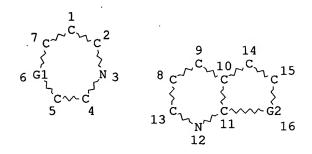
L6 39 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[3,2-b]pyridine, 3-(4-fluorophenyl)-1-[3-(hexahydro-1H-1,4-diazepin-1-yl)propyl]-2-(4-pyridinyl)-, tris(trifluoroacetate) (9CI)
MF C26 H28 F N5 . 3 C2 H F3 O2

CM 1

CM 2

ALL ANSWERS HAVE BEEN SCANNED



VAR G1=C/N
VAR G2=O/S/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1 8
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

=> s 11 ful FULL SEARCH INITIATED 13:26:04 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 167090 TO ITERATE

100.0% PROCESSED 167090 ITERATIONS 173 ANSWERS SEARCH TIME: 00.00.01

L3 173 SEA SSS FUL L1

=> d scan

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 4-[6-(hexahydro-1H-1,4-diazepin-1-yl)-5-(1-pyrrolidinyl)pyrazinyl]- (9CI)

MF C20 H25 N7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):172

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-(hexahydro-4-phenyl-1H-1,4-diazepin-1-yl)-6-methyl- (9CI)

MF C20 H23 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4-

[(dimethylamino)carbonyl]phenyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C22 H26 N6 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 4-(4-acetylhexahydro-1H-1,4-diazepin-1-yl)-3-amino- (9CI)

MF C15 H19 N5 O2 S

L3

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(2,3,5,6-IN

tetrafluoro-4-pyridinyl)-1H-1,4-diazepin-1-yl]- (9CI) C18 H16 F4 N6 O S

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4-

(dimethylamino)phenyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

C21 H26 N6 O S MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(2-chlorophenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C19 H20 C1 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, 1-acetyl-4-[6-(5-chloro-1H-pyrrolo[2,3-b]pyridin-3-yl)-4cyano-2-pyridinyl]hexahydro- (9CI)

MF C20 H19 C1 N6 O

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

1H-1,4-Diazepine, 1-acetylhexahydro-4-[6-(5-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)-2-pyridinyl]- (9CI) C20 H23 N5 O IN

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN L3

1H-Pyrrolo[2,3-b]pyridine, 2-[6-[3-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)propoxy]-5-methoxy-1-methyl-1H-indol-3-yl]- (9CI) IN

C26 H33 N5 O2 MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, 4-[3-amino-2-(aminocarbonyl)-4-(3-furanyl)thieno[2,3-b]pyridin-6-yl]hexahydro-, 1,1-dimethylethyl ester
(9CT)

MF C22 H27 N5 O4 S

$$t-BuO-C N N S C-NH2$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, 4-[1-[2-amino-6-[[3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4-yloxy)phenyl]amino]-4-pyrimidinyl]-3azetidinyl]hexahydro-, 1,1-dimethylethyl ester (9CI)

MF C30 H36 F N9 O3

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 3-(hexahydro-1-methyl-1H-azepin-4-yl)-1-(1-naphthalenylsulfonyl)- (9CI)

MF C24 H25 N3 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C19 H21 N5 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carbothioic acid, 3-amino-5-[2-(hexahydro-4-methyl1H-1,4-diazepin-1-yl)ethoxy]-4,6-dimethyl-, O-(1,1-dimethylethyl) ester
(9CI)

MF C22 H34 N4 O2 S2

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4-[3-(dimethylamino)-3-oxopropyl]phenyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C24 H30 N6 O2 S

$$\begin{array}{c|c} O \\ \parallel \\ Me_2N-C-CH_2-CH_2 \\ \hline \\ N \\ \hline \\ N \\ \hline \\ N \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(1-hydroxyethyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF C21 H25 N5 O2 S

L3 · 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4-(1,1- $^{\circ}$ dimethylethyl)phenyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C23 H29 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-IN

(phenylmethoxy)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

C26 H27 N5 O2 S MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(3-methylphenyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H23 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, 1-acetylhexahydro-4-[4-(1H-pyrrolo[2,3-b]pyridin-3-yl)-2pyrimidinyl]- (9CI)

MF C18 H20 N6 O

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, 4-[6-(5-chloro-1H-pyrrolo[2,3-

b]pyridin-3-yl)-2-pyridinyl]hexahydro-, ethyl ester (9CI)

MF C20 H22 C1 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine-5-carboxamide, 3-[2-(4-acetylhexahydro-1H-1,4-diazepin-1-yl)-4-pyrimidinyl]- (9CI)

MF C19 H21 N7 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN Cyclohexanecarboxamide, N-[3-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]-1H-IN pyrrolo[2,3-b]pyridin-5-yl]- (9CI)

MF C20 H27 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Propanamide, N-[4-[7-[(2,6-difluorophenyl)methyl]-3-[(hexahydro-1H-azepin-methyl]-3-[(hexahy1-yl)methyl]-4,7-dihydro-5-(2-methyl-1-oxopropyl)-4-oxothieno[2,3b]pyridin-2-yl]phenyl]-2-methyl- (9CI)

MF C35 H39 F2 N3 O3 S

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2007 ACS on STN L3 173 ANSWERS

IN Thieno[2,3-b]pyridine-2-carboxylic acid, 6-(hexahydro-1H-azepin-1-yl)-4-(trifluoromethyl)-, methyl ester (9CI)

MF C16 H17 F3 N2 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[2,3-b]pyridine-2-carboxamide, 3-[[(hexahydro-1H-azepin-1-yl)carbonyl]amino]-

MF C15 H18 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Propanediamide, N-[3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4-yloxy)phenyl]-N'-(hexahydro-1H-azepin-1-yl)- (9CI)

MF C22 H24 F N5 O3

PAGE 1-A

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4[(dimethylamino)carbonyl]-2-thiazolyl]hexahydro-1H-1,4-diazepin-1-yl](9CI)

MF C19 H23 N7 O2 S2

$$\begin{array}{c|c} O & & \\ \parallel & & \\ Me_2N-C & & \\ N & & S & \\ \hline & N & & \\ N & & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(2-oxopropyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF C22 H25 N5 O2 S

- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(2-thiazolyl)1H-1,4-diazepin-1-yl]- (9CI)
- MF C16 H18 N6 O S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(4-ethoxyphenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)
- MF C21 H25 N5 O2 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(4-fluoro-3-

methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H22 F N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(phenylmethyl)1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H23 N5 O S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine-5-carboxylic acid, 3-[6-(4-acetylhexahydro-1H-

1,4-diazepin-1-yl)-2-pyridinyl]- (9CI)

MF C20 H21 N5 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN lH-1,4-Diazepine, 1-acetylhexahydro-4-[4-(5-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)-2-pyrimidinyl]- (9CI)

MF C19 H22 N6 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 2-[1-[2-[hexahydro-4-[3-(1-pyrrolidinyl)propyl]-1H-1,4-diazepin-1-yl]ethyl]-5,6-dimethoxy-1H-indol-3-yl]- (9CI)

MF C31 H42 N6 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine-3-carboxaldehyde, 2-(hexahydro-1H-1,4-diazepin-1-yl)-1-phenyl-, mono(trifluoroacetate) (9CI)

MF C19 H20 N4 O . C2 H F3 O2

CM 1

CM 2

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-(3-aminohexahydro-1H-azepin-1-yl)-4-propyl- (9CI)

MF C17 H25 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[2,3-b]pyridine-2-carboxamide, 3-[[[2-[(hexahydro-1H-azepin-1-yl)carbonyl]-4-morpholinyl]carbonyl]amino]-6-methyl-

MF C21 H27 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 4-[6-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-

5-(1-pyrrolidinyl)pyrazinyl]-, dihydrochloride (9CI)

MF C21 H27 N7 . 2 C1 H

●2 HC1

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[3,4-dihydro-4-(hydroxyimino)-2H-1-benzopyran-7-yl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI) L3 IN MF C22 H24 N6 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN L3

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(3-hydroxypropyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI) IN

C22 H27 N5 O2 S MF

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN L3

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-(hexahydro-1H-1,4-diazepin-IN

1-yl)-, dihydrochloride (9CI) C13 H17 N5 O S . 2 Cl H MF

●2 HC1

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN L3

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-IN

(trifluoromethoxy)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

C20 H20 F3 N5 O2 S MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(methylsulfonyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF. C20 H23 N5 O3 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(4-

chlorophenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C19 H20 C1 N5 O S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Propanamide, N-[3-[6-(4-acetylhexahydro-1H-1,4-diazepin-1-yl)-2-pyridinyl]-

1H-pyrrolo[2,3-b]pyridin-5-yl]- (9CI)

MF C22 H26 N6 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[4-(5-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)-2-pyrimidinyl]-, propyl ester (9CI)

pyrioto(2,5 b)pyriotin 5 yr, 2 pyrimiotinyr, propyr ester (.

MF C21 H26 N6 O3

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 2-[6-[2-(hexahydro-4-methyl-1H-1,4-diazepin-1yl)ethoxy]-5-methoxy-1-methyl-1H-indol-3-yl]- (9CI)

MF C25 H31 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, 4-[3-amino-2-(aminocarbonyl)-4-(2furanyl)thieno[2,3-b]pyridin-6-yl]hexahydro-, 1,1-dimethylethyl ester (9CI)

MF C22 H27 N5 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-(4-aminohexahydro-1H-azepin-1-yl)-4-propyl- (9CI)

MF C17 H25 N5 O S

$$H_2N$$
 N
 S
 $C-NH_2$
 NH_2

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 1-(phenylsulfonyl)-3-(2,3,6,7-tetrahydro-1methyl-1H-azepin-4-yl)- (9CI)

MF C20 H21 N3 O2 S

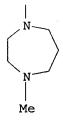
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine-4-carboxamide, N-[4-[5-fluoro-6-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-1H-benzimidazol-2-yl]-9H-fluoren-9-yl]- (9CI)

MF C34 H30 F N7 O

PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzeneacetamide, 3-[(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)sulfonyl]-N-[4-(1H-pyrrolo[2,3-b]pyridin-3-yl)-2-thiazolyl]- (9CI)

MF C24 H26 N6 O3 S2

$$\begin{array}{c|c} & & & \\ & & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4-[2-(dimethylamino)-2-oxoethyl]phenyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C23 H28 N6 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(5-methyl-2-pyridinyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C19 H22 N6 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(1-methylethoxy)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF C22 H27 N5 O2 S

L3173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(3chlorophenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

C19 H20 C1 N5 O S MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-IN

(methylthio)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

C20 H23 N5 O S2 MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 3-[2-(hexahydro-1H-1,4-diazepin-1-yl)-4pyrimidinyl]- (9CI)

MF C16 H18 N6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, 4-[6-(5-chloro-1H-pyrrolo[2,3-b]pyridin-3-yl)-2-pyridinyl]hexahydro-, methyl ester (9CI)

MF C19 H20 Cl N5 O2

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 2-[1-[3-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)propyl]-5,6-dimethoxy-1H-indol-3-yl]-1-[(4-methylphenyl)sulfonyl]-,
 trifluoroacetate (9CI)

MF C33 H39 N5 O4 S . \times C2 H F3 O2

CM 1

PAGE 1-A

CM 2

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Propanamide, N-[3-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]-1H-

pyrrolo[2,3-b]pyridin-5-yl]-2,2-dimethyl- (9CI)

MF C18 H25 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2,4-Pyrimidinediamine, N4-[3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4-

yloxy)phenyl]-6-[3-(hexahydro-1H-1,4-diazepin-1-yl)-1-azetidinyl]- (9CI)

MF C25 H28 F N9 O

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 1-[(2,3-dichlorophenyl)sulfonyl]-3-(2,3,6,7-tetrahydro-1-methyl-1H-azepin-4-yl)- (9CI)

MF C20 H19 C12 N3 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C13 H15 C1 N4 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, hexahydro-1-[imino[3-[3-(2-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridin-5-yl]phenyl]methyl]-4-methyl- (9CI)

MF C27 H29 N5 O

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Ethanethioic acid, S-[4-[4-[3-amino-2-(aminocarbonyl)thieno[2,3-b]pyridin-4-yl]hexahydro-1H-1,4-diazepin-1-yl]phenyl] ester (9CI)

4-yijnexanydro-in-i,4-diazepin-i-yijpnenyi

MF C21 H23 N5 O2 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-[(2-methyl-1,3-dioxolan-2-yl)methyl]phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF C24 H29 N5 O3 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(3-pyridinyl)1H-1,4-diazepin-1-yl]- (9CI)

MF C18 H20 N6 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(4-bromophenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C19 H20 Br N5 O S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(3-methoxyphenyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H23 N5 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, 4-[3-amino-2-(aminocarbonyl)thieno[2,3-b]pyridin-4-yl]hexahydro-, 1,1-dimethylethyl ester (9CI)

MF C18 H25 N5 O3 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine-5-carboxamide, 3-[6-(4-acetylhexahydro-1H-1,4-diazepin-1-yl)-2-pyridinyl]-N-[3-(4-methyl-1-piperazinyl)propyl]- (9CI)

MF C28 H38 N8 O2

$$N = (CH_2)_3 - NH - C$$

$$N = N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 5-chloro-3-[2-(hexahydro-1H-azepin-1-yl)-4pyrimidinyl]- (9CI)

MF C17 H18 C1 N5

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 2-[1-[2-(hexahydro-4-methyl-1H-1,4-diazepin-1yl)ethyl]-5,6-dimethoxy-1H-indol-3-yl]- (9CI)

MF C25 H31 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN lh-Pyrrolo[2,3-b]pyridine-3-carboxaldehyde, 2-(hexahydro-1H-1,4-diazepin-1-yl)-1-phenyl- (9CI)

MF C19 H20 N4 O

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 6-(4-acetylhexahydro-1H-1,4-diazepin-1-yl)-3-amino-4-propyl- (9CI)

MF C18 H25 N5 O2 S

REGISTRY COPYRIGHT 2007 ACS on STN L3 173 ANSWERS

Furo[2,3-b]pyridine-2-carboxamide, 3-[[[3-[(hexahydro-1H-azepin-1-IN

yl) carbonyl]-1-piperidinyl]carbonyl]amino]-6-methyl-

C22 H29 N5 O4 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2007 ACS on STN L3

Pyrazinamine, 3-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-5-(1H-IN

pyrrolo[2,3-b]pyridin-4-yl)- (9CI)

C17 H21 N7 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2007 ACS on STN L3 173 ANSWERS

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(6-IN benzoxazolyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

C20 H20 N6 O2 S MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[3-(2-hydroxyethyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF C21 H25 N5 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(4-pyridinyl)1H-1,4-diazepin-1-yl]- (9CI)

MF C18 H20 N6 O S

- REGISTRY COPYRIGHT 2007 ACS on STN L3 173 ANSWERS
- Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[3-IN (trifluoromethyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)
- MF C20 H20 F3 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3
- 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(2,3-dihydro-1,4-IN benzodioxin-6-yl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI) C21 H23 N5 O3 S
- MF

L3 173 ANSWERS

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(4-nitrophenyl)-1H-1,4-diazepin-1-yl]- (9CI) IN

MF C19 H20 N6 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN L3

Acetamide, N-[3-[6-(4-acetylhexahydro-1H-1,4-diazepin-1-yl)-2-pyridinyl]-IN 1H-pyrrolo[2,3-b]pyridin-5-yl]- (9CI)

C21 H24 N6 O2 MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[4-(5-methoxy-1H-

pyrrolo[2,3-b]pyridin-3-yl)-2-pyrimidinyl]-, ethyl ester (9CI)

MF C20 H24 N6 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, hexahydro-1-[[[5-methoxy-1-methyl-3-(1H-pyrrolo[2,3-

b]pyridin-2-yl)-1H-indol-6-yl]oxy]acetyl]-4-methyl- (9CI)

MF C25 H29 N5 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carbonitrile, 3-amino-6-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-4-propyl- (9CI)

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-(hexahydro-4-hydroxy-1H-azepin-1-yl)-4-propyl- (9CI)

MF C17 H24 N4 O2 S

HO N S
$$C-NH_2$$
 $N+1$
 $N+2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C20 H23 N3 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 4-[6-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)5-(1-pyrrolidinyl)pyrazinyl]- (9CI)

MF C21 H27 N7

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-(hexahydro-1H-1,4-diazepin-1-yl)- (9CI)

MF C13 H17 N5 O S

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(4-morpholinylcarbonyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF C24 H28 N6 O3 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(6-chloro-3-pyridazinyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C17 H18 C1 N7 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(4-methyl-3-nitrophenyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H22 N6 O3 S

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ N & &$$

- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(4-IN methylphenyl)-1H-1,4-diazepin-1-yl]- (9CI)
- MF C20 H23 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3
- 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-IN (trifluoromethyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)
- MF C20 H20 F3 N5 O S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, 1-acetylhexahydro-4-[6-(1H-pyrrolo[2,3-b]pyridin-3-yl)-4pyrimidinyl]- (9CI)

MF C18 H20 N6 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

M1 C27 M34 NO O2

Relative stereochemistry.

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C33 H39 N5 O4 S

CI COM

PAGE 1-A

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-(hexahydro-1H-azepin-1-yl)4-(3-piperidinyl)- (9CI)

MF C19 H27 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Azepine, 1-[(3-amino-4,6-dimethylthieno[2,3-b]pyridin-2yl)carbonyl]hexahydro- (9CI)

MF C16 H21 N3 O S

Me
$$N \longrightarrow S \longrightarrow C \longrightarrow N$$
 NH_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN lH-Pyrrolo[2,3-b]pyridine, 3-[hexahydro-1-(2-phenylethyl)-1H-azepin-4-yl]l-(1-naphthalenylsulfonyl)- (9CI)

MF C31 H31 N3 O2 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C19 H20 C1 N5 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Phenol, 2-[(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)methyl]-4-[3-(2-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridin-5-yl]- (9CI)

MF C27 H30 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 4-[4-(5-acetyl-2-pyridinyl)hexahydro1H-1,4-diazepin-1-yl]-3-amino- (9CI)
MF C20 H22 N6 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(1-oxopropyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)
MF C22 H25 N5 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 4-[4-(4-acetylphenyl)hexahydro-1H-1,4-diazepin-1-yl]-3-amino- (9CI)

MF C21 H23 N5 O2 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(3-chloro-4-fluorophenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C19 H19 C1 F N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(2-methoxyphenyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H23 N5 O2 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C14 H18 N4 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine-5-carboxamide, 3-[6-(4-acetylhexahydro-1H-1,4-diazepin-1-yl)-2-pyridinyl]-N-[2-(4-morpholinyl)ethyl]- (9CI)

MF C26 H33 N7 O3

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, 1-acetyl-4-[4-(5-chloro-1H-pyrrolo[2,3-b]pyridin-3-yl)-2pyrimidinyl]hexahydro- (9CI)

MF C18 H19 Cl N6 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Hexanamide, 2-ethyl-N-[3-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]-1Hpyrrolo[2,3-b]pyridin-5-yl]- (9CI)

MF C21 H31 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Azepine, 1-[[3-amino-6-(4-chlorophenyl)-4-(trifluoromethyl)thieno[2,3-b]pyridin-2-yl]carbonyl]hexahydro- (9CI)

MF C21 H19 C1 F3 N3 O S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-4-propyl- (9CI)

MF C17 H25 N5 O S

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Me} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[2,3-b]pyridine-2-carboxamide, 3-[[[3-[(hexahydro-1H-azepin-1-

yl)carbonyl]-1-piperidinyl]carbonyl]amino]-

MF C21 H27 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C22 H28 N4 O S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(2,3-dihydro-2-methyl-1oxo-1H-isoindol-5-yl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C22 H24. N6 O2 S

$$\begin{array}{c|c} & & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(2-methoxyethyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF C22 H27 N5 O2 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(2-pyridinyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C18 H20 N6 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(3,4-difluorophenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C19 H19 F2 N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(3-fluoro-4-methylphenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H22 F N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS ' REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(4-methoxyphenyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H23 N5 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2-Propenamide, N-[3-[6-(4-acetylhexahydro-1H-1,4-diazepin-1-yl)-2-

pyridinyl]-1H-pyrrolo[2,3-b]pyridin-5-yl]- (9CI)
C22 H24 N6 O2

$$H_2C = CH - C - NH$$

$$N$$

$$N$$

$$N$$

$$N$$

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-1,4-Diazepine, 1-(ethylsulfonyl)hexahydro-4-[4-(5-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)-2-pyrimidinyl]- (9CI)
MF C19 H24 N6 O3 S

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 2-[1-[3-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)propyl]-5,6-dimethoxy-1H-indol-3-yl]-, trifluoroacetate (9CI)

MF C26 H33 N5 O2 . \times C2 H F3 O2

CM 1

CM 2

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 3-[4-(2,3-difluorophenyl)-4H-1,2,4-triazol-3-yl]-5-[6-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-3-pyridinyl]- (9CI)

MF C26 H24 F2 N8

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-(hexahydro-5-oxo-1H-1,4-diazepin-1-yl)-4-propyl- (9CI)

MF C16 H21 N5 O2 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, 1-[[3-[(3,4-dihydro-3-oxo-2H-1,4-benzothiazin-2-ylidene)methyl]-1H-pyrrolo[2,3-b]pyridin-1-yl]acetyl]hexahydro-4-methyl(9CI)

MF C24 H25 N5 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[3-(1-pyrrolidinyl)-6-(1H-pyrrolo[2,3-b]pyridin-4-yl)pyrazinyl]-, 1,1-dimethylethyl ester (9CI)

MF C25 H33 N7 O2

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4[(dimethylamino)carbonyl]phenyl]hexahydro-1H-1,4-diazepin-1-yl]-6-methyl(9CI)

MF C23 H28 N6 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4-(1-azetidinylcarbonyl)phenyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C23 H26 N6 O2 S

- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(methylsulfonyl)-1H-1,4-diazepin-1-yl]- (9CI)
- MF C14 H19 N5 O3 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(4-quinazolinyl)-1H-1,4-diazepin-1-yl]- (9CI)
- MF C21 H21 N7 O S

$$H_2N$$
 H_2N
 O

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(4-fluorophenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C19 H20 F N5 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(4-cyanophenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H20 N6 O S

L3

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN 4-Pyridinecarbonitrile, 2-(5-chloro-1H-pyrrolo[2,3-b]pyridin-3-yl)-6-IN (hexahydro-1H-1,4-diazepin-1-yl)- (9CI)

MF C18 H17 C1 N6

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IN 1H-1,4-Diazepine, 1-acetyl-4-[6-(5-fluoro-1H-pyrrolo[2,3-b]pyridin-3-yl)-2pyridinyl]hexahydro- (9CI)

C19 H20 F N5 O MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN lH-Pyrrolo[2,3-b]pyridine, 2-[6-[2-[2-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)ethoxy]-5-methoxy-1-methyl-1H-indol-3-yl]- (9CI)

MF C27 H35 N5 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 1-Piperidinecarboxylic acid, 3-[3-amino-2-(aminocarbonyl)-6-(hexahydro-1H-azepin-1-yl)thieno[2,3-b]pyridin-4-yl]-, 1,1-dimethylethyl ester (9CI)

MF C24 H35 N5 O3 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2,4-Pyrimidinediamine, N4-[3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4yloxy)phenyl]-6-[3-(hexahydro-1H-1,4-diazepin-1-yl)-1-azetidinyl]-,
hydrochloride (9CI)

MF C25 H28 F N9 O . x Cl H

•x HCl

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 1-(8-quinolinylsulfonyl)-3-(2,3,6,7-tetrahydro-1-methyl-1H-azepin-4-yl)- (9CI)

MF C23 H22 N4 O2 S

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L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED MF C20 H20 N6 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Phenol, 2-[(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)methyl]-5-[3-(2-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridin-5-yl]- (9CI)

MF C27 H30 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-[4-[2-

(dimethylamino)ethyl]phenyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI)

MF C23 H30 N6 O S

$$\begin{array}{c|c} \text{Me}_2\text{N}-\text{CH}_2-\text{CH}_2 \\ \hline \\ \text{N} \\ \hline \\ \text{N} \\ \end{array}$$

- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- MF C21 H24 N6 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(4-ethylphenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)
- MF C21 H25 N5 O S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(3nitrophenyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C19 H20 N6 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(methylsulfinyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI) IN

C20 H23 N5 O2 S2 MF

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, 1-acetyl-4-[4-(5-cyano-1H-pyrrolo[2,3-b]pyridin-3-yl)-2-pyrimidinyl]hexahydro- (9CI)

MF C19 H19 N7 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, 1-acetylhexahydro-4-[6-(5-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)-2-pyridinyl]- (9CI)

MF C20 H23 N5 O2

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-1,4-Diazepine, 1-acetylhexahydro-4-[4-[5-(3-pyridinyl)-1H-pyrrolo[2,3-b]pyridin-3-yl]-2-pyrimidinyl]- (9CI)

MF C23 H23 N7 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 · 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzamide, N-[3-[(hexahydro-1H-1,4-diazepin-1-yl)carbonyl]-1H-pyrrolo[2,3-b]pyridin-5-yl]-2-methoxy- (9CI)

MF C21 H23 N5 O3

$$\begin{array}{c|c} O & & H & O \\ \hline C - NH & & N & C - N & NH \\ \hline OMe & & & & \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 1H-Pyrrolo[2,3-b]pyridine-2-carboxamide, 6-chloro-N-[(1S)-1-[(4-fluorophenyl)methyl]-2-(hexahydro-5-oxo-1H-1,4-diazepin-1-yl)-2-oxoethyl](9CI)

MF C22 H21 C1 F N5 O3

Absolute stereochemistry.

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IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-(hexahydro-1H-1,4-diazepin-1-yl)-4-propyl- (9CI)

MF C16 H23 N5 O S

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L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Furo[2,3-b]pyridine-2-carboxamide, 3-[[[(3R)-3-(hexahydro-1H-azepin-1-yl)1-pyrrolidinyl]carbonyl]amino]-

MF C19 H25 N5 O3

Absolute stereochemistry.

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C23 H30 N4 O S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 4-[4-(4-acetyl-2-thiazolyl)hexahydro-

1H-1,4-diazepin-1-yl]-3-amino- (9CI)

MF C18 H20 N6 O2 S2

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IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-[4-(2-

hydroxyethyl)phenyl]-1H-1,4-diazepin-1-yl]- (9CI)

MF C21 H25 N5 O2 S

- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(6-methoxy-3-pyridinyl)-1H-1,4-diazepin-1-yl]- (9CI)
- MF C19 H22 N6 O2 S

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- L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[4-(3,4
 - dimethylphenyl)hexahydro-1H-1,4-diazepin-1-yl]- (9CI)
- MF C21 H25 N5 O S

Me Me NH2
$$C-NH_2$$

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-[hexahydro-4-(2-methylphenyl)-1H-1,4-diazepin-1-yl]- (9CI)

MF C20 H23 N5 O S

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IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-4-(hexahydro-4-phenyl-1H-1,4-diazepin-1-yl)- (9CI)

MF C19 H21 N5 O S

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IN 2-Propenamide, N-[3-[6-[4-(cyanoacetyl)hexahydro-1H-1,4-diazepin-1-yl]-2-

pyridinyl]-1H-pyrrolo[2,3-b]pyridin-5-yl]- (9CI)
MF C23 H23 N7 O2

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IN 1H-1,4-Diazepine, hexahydro-1-[4-(5-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)2-pyrimidinyl]-4-(methylsulfonyl)- (9CI)

MF C18 H22 N6 O3 S

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrolo[2,3-b]pyridine, 2-[1-[3-(hexahydro-4-methyl-1H-1,4-diazepin-1yl)propyl]-5,6-dimethoxy-1H-indol-3-yl]- (9CI)

MF C26 H33 N5 O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 1H-1,4-Diazepine-1-carboxylic acid, 4-(3-formyl-1-phenyl-1H-pyrrolo[2,3-b]pyridin-2-yl)hexahydro-, 1,1-dimethylethyl ester (9CI)

MF C24 H28 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-[4-(aminocarbonyl)hexahydro-1H-1,4-diazepin-1-yl]-4-propyl- (9CI)

MF C17 H24 N6 O2 S

L3 173 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Propanamide, N-[4-[7-[(2,6-difluorophenyl)methyl]-3-[(hexahydro-1H-azepin-1-yl)methyl]-4,7-dihydro-5-(2-methyl-1-oxopropyl)-4-oxothieno[2,3-b]pyridin-2-yl]phenyl]-2-methyl-, monohydrobromide (9CI)

MF C35 H39 F2 N3 O3 S . Br H

HBr

ALL ANSWERS HAVE BEEN SCANNED